

The ^4He tetramer ground state in the Faddeev-Yakubovsky

differential equations formalism

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Abstract

The characteristics of the four ^4He atom cluster are investigated using the differential equations for Yakubovsky components. Binding energy, mean-square radius and density function are calculated for the ground state. The spatial properties of the cluster and its subsystems are studied.

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I. INTRODUCTION

In the present work clusters of three and four helium atoms are investigated. In recent years such systems had attracted growing attention due to development of experimental techniques allowing to observe and to study two and three-particle Helium clusters^{1,2} and as a result of theoretical developments which made possible the construction of realistic pair potentials *ab initio*³⁻⁸.

The last two decades have been significant progress in the investigation of few-body systems. This progress rests on the development of new techniques for solving Faddeev and Yakubovsky (FY) equations^{9,10,13,14} for wave function components and growing power of computer facilities that allowed to reach higher accuracy in the branch of Monte-Carlo techniques. Though equivalent to Schrödinger equation the system of FY equations has significant advantages over the Schrödinger one. These advantages have their origin in a proper choice of wave function decomposition into the components. The equations are constructed so that only one pair potential enters the equation for a particular component provided that the interaction in the system is given in terms of pairwise potentials. This nice feature leads to very simple boundary conditions for the components and simplifies their numerical approximation significantly. Traditionally Yakubovsky equations are used in nuclear physics¹¹⁻¹⁸. In spite of strong mathematical background and effective numerical techniques developed for Faddeev and Yakubovsky equations only a few papers devoted to molecular physics exploiting the technique of Faddeev or Yakubovsky equations are known. Most of them are devoted to a system of Helium trimer¹⁹⁻²³. No four-body calculations of molecular systems based on Yakubovsky equations are known to the authors up to now. The aim of the present paper is to take the first step towards wider exploiting the rigorous and effective technique of Yakubovsky equations in molecular and chemical physics.

The numerical scheme exploited in this paper to solve differential Yakubovsky equations is the cluster reduction method (CRM)¹⁸ which opens a way to construct small subspaces containing solutions of the equations. This method developed and repeatedly applied to the

problems of nuclear physics has been employed in the present paper to perform a calculation of bound state characteristics of a system of four helium atoms. The method allows to obtain not only the estimations for the binding energy of a four particle system but also the wave function of the system using computer resources economically. Another important advantage of CRM is applicability of the method to model-free calculations of multichannel reactions in a system of four particles^{15,17,18}. Being applied to systems of four helium atoms it can be used to calculate the reaction rates for $\text{He}_2 + \text{He}_2 \rightarrow \text{He}_3 + \text{He}$ and $\text{He}_2 + \text{He}_2 \rightarrow \text{He}_3^* + \text{He}$ processes. Calculating *s*-wave model of He_4 tetramer in this paper we make a step towards investigation of reactions in systems of four atoms on the base of strongly grounded mathematically correct methods.

This paper contains three additional sections and a conclusion. In section 2 the model is described and the main equations are given. In the section 3 the method of solution is presented. Section 4 contains the results of numerical calculations.

II. FORMALISM

The calculations presented here were performed in the framework of differential Yakubovsky equations (DYE) for four particles in configuration space. The formalism of differential Yakubovsky equations was developed by S.P.Merkuriev and S.L.Yakovlev¹⁰. Here we only give a brief description of these equations touching upon the approximations that we use and emphasizing the advantages of using the DYE instead of the Shrödinger equation in investigations of bound states of four particles. Detailed and sound description of the equations and asymptotic boundary conditions can be found in the original paper¹² and in more detail in the book by Merkuriev and Faddeev⁹.

When considering a system of four particles it is convenient to use Jacobi coordinates. For identical particles there are two types of Jacobi coordinates, which correspond to different partitions of the four particle system into subsystems. The first type corresponds to the partitioning into a three-particle cluster and one separate particle (3+1 type). The second

one corresponds to the partitioning into two-particle clusters (2+2 type). The explicit expressions for the Jacobi coordinates through the particle coordinate vectors \mathbf{r}_k , $k = 1, 2, 3, 4$ are given by the formulas

$$\begin{aligned}\mathbf{x}_{2,1} &= \mathbf{r}_2 - \mathbf{r}_1 , \\ \mathbf{y}_{3,21} &= (\mathbf{r}_1 + \mathbf{r}_2)/2 - \mathbf{r}_3 , \\ \mathbf{z}_{4,321} &= (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)/3 - \mathbf{r}_4 ,\end{aligned}\tag{1}$$

for the first type of coordinates and

$$\begin{aligned}\mathbf{x}_{1,2} &= \mathbf{r}_2 - \mathbf{r}_1 , \\ \mathbf{y}_{3,4} &= \mathbf{r}_4 - \mathbf{r}_3 , \\ \mathbf{z}_{34,12} &= (\mathbf{r}_1 + \mathbf{r}_2)/2 - (\mathbf{r}_3 + \mathbf{r}_4)/2 ,\end{aligned}\tag{2}$$

for the second one. The Jacobi coordinates for partitions of the same type but with different distribution of particles among the clusters can be obtained by cyclic permutations of the subscripts enumerating the particles in (1) and (2).

Suppose the Hamiltonian of a system of four particles has the form

$$H = H_0 + \sum_{\alpha} V(\mathbf{x}_{\alpha}) ,\tag{3}$$

where H_0 is the Hamiltonian of the system of free particles, α stands for two-particle subsystems of the four-body system and $V(\mathbf{x}_{\alpha})$ is the potential of the interaction in the pair with index α . For the systems of identical particles the wave function Ψ can be expressed in terms of two Yakubovsky components U^k , $k=1,2$. U^1 corresponds to the partition 3+1 and U^2 corresponds to the partition 2+2. The expression of the total wave function of the system in terms of Yakubovsky components reads^{12,18}

$$\begin{aligned}\Psi &= (I + P^+ + P^+P^+ + P^-)(I + P_4^+ + P_4^-)U^1 + \\ &+ (I + P_1^+ + P_1^-)(I + P^+P^+)U^2 .\end{aligned}\tag{4}$$

Here P^+ (P^-) are the operators of cyclic (anticyclic) permutations of four particles, P_i^{\pm} correspond to cyclic permutations of three particles with fixed i -th particle. The Yakubovsky components U^1 and U^2 satisfy the following set of the equations¹²:

$$\begin{aligned}
(H_0 + V(\mathbf{x}) - E) U^1 + V(\mathbf{x})(P_4^+ + P_4^-) U^1 &= \\
&= - V(\mathbf{x}) \left((P_1^+ + P^+) U^1 + (P_1^+ + P_4^+) U^2 \right) , \\
(H_0 + V(\mathbf{x}) - E) U^2 + V(\mathbf{x})(P^+ P^+) U^2 &= \\
&= - V(\mathbf{x})(P^+ + P_1^+) P^+ U^1 .
\end{aligned} \tag{5}$$

Here we have omitted the subsystem index α in the notation of coordinates \mathbf{x} since all the particles are identical. The advantages of using the equations for Yakubovsky components instead of solving directly the Shrödinger equation come from better localization of the interaction in configuration space. In the special case of identical particles the DYE can be written in term of the interaction potential of only one pair. As a result the numerical approximation of the Yakubovsky components is a much easier problem than the approximation of the wave function. Detailed discussion of Yakubovsky equations can be found in the monograph by Merkuriev and Faddeev⁹.

We solve the equations for Yakubovsky components in the s -wave approximation in which the angular momenta of the system of four atoms and all its subsystems are set to zero. The s -wave equations for Yakubovsky components \mathcal{U}^k , $k=1,2$ have the following form⁹

$$\begin{aligned}
(h_0^1 + v(x) - \varepsilon) \mathcal{U}^1(x, y, z) + v(x) \int_{-1}^1 dv \frac{xy}{x_1 y_1} \mathcal{U}^1(x_1, y_1, z_1) &= \\
= -\frac{1}{2} v(x) \int_{-1}^1 du \int_{-1}^1 dv \left(\frac{xyz}{x_2 y_2 z_2} \mathcal{U}^1(x_2, y_2, z_2) + \right. \\
&\quad \left. + \frac{xyz}{x_3 y_3 z_3} \mathcal{U}^2(x_3, y_3, z_3) \right) , \\
(h_0^2 + v(x) - \varepsilon) \mathcal{U}^2(x, y, z) + v(x) \mathcal{U}^2(y, x, z) &= \\
= -\frac{1}{2} v(x) \int_{-1}^1 du \frac{xyz}{x_4 y_4 z_4} \mathcal{U}^1(x_4, y_4, z_4) ,
\end{aligned} \tag{6}$$

where $x = |\mathbf{x}|$, $y = |\mathbf{y}|$, $z = |\mathbf{z}|$,

$$\begin{aligned}
h_0^1 &= -(\partial_x^2 + \frac{3}{4} \partial_y^2 + \frac{2}{3} \partial_z^2), \\
h_0^2 &= -(\partial_x^2 + \partial_y^2 + \frac{1}{2} \partial_z^2),
\end{aligned}$$

$v(x)$ is s-wave component of the pair potential $V(x)$. The coordinates $x_i, y_i, z_i, i=1,2,3,4$ in the kernels of the equations (6) are defined by the following relations:

$$\begin{aligned}
x_1 &= \left(\frac{x^2}{4} + y^2 + xyv \right)^{1/2}, & y_1 &= \left(\left(\frac{3}{4}x \right)^2 + \frac{y^2}{4} - \frac{3}{4}xyv \right)^{1/2}, \\
x_2 &= x_1, & x_3 &= x_1, & x_4 &= y, \\
y_2 &= \left(\left(\frac{y_1}{3} \right)^2 + z^2 + \frac{2}{3}y_1zu \right)^{1/2}, & z_2 &= \left(\left(\frac{8}{9}y_1 \right)^2 + \frac{z^2}{9} - \frac{16}{27}y_1zu \right)^{1/2}, \\
y_3 &= \left(\left(\frac{2}{3}y_1 \right)^2 + z^2 + \frac{4}{3}y_1zu \right)^{1/2}, & z_3 &= \left(\left(\frac{2}{3}y_1 \right)^2 + \frac{z^2}{4} - \frac{2}{3}y_1zu \right)^{1/2}, \\
y_4 &= \left(\left(\frac{x}{2} \right)^2 + z^2 - xzu \right)^{1/2}, & z_4 &= \frac{2}{3} \left(x^2 + z^2 + 2xzu \right)^{1/2}.
\end{aligned}$$

III. METHOD OF SOLUTION

The differential equations for the Yakubovsky components (6) are solved using the cluster reduction method (CRM). This method has been developed and applied before^{15,17,18} to calculate the characteristics of bound states and low-energy scattering of systems of three and four particles. The cluster reduction method reduces considerably the computational difficulties when solving DYE numerically. In the framework of the CRM Faddeev (Yakubovsky) components are decomposed in terms of the eigenfunctions of the Hamiltonians of two (three) particles subsystems. As a result of the projection onto the elements of a biorthogonal basis we obtain the set of equations corresponding to the relative motion of clusters. A brief summary of the CRM from Yakovlev and Filikhin¹⁸ is given below. The Yakubovsky components $\mathcal{U}^i, i=1,2$ are written in the following form

$$\mathcal{U}^i(x, y, z) = \sum_{l=0}^{\infty} \phi_l^i(x, y) F_l^i(z), \quad i = 1, 2. \quad (7)$$

In the Eq. (7) the basic functions ϕ_l^i are the solutions of s -wave Faddeev equations for subsystems of types $3 + 1$ ($i = 1$) and $2 + 2$ ($i = 2$):

$$\begin{aligned}
\{-\partial_x^2 - \frac{3}{4}\partial_y^2 + v(x)\}\phi_l^1(x, y) + v(x) \int_{-1}^1 dv \frac{xy}{x_1 y_1} \phi_l^1(x_1, y_1) = \\
= \varepsilon_1^l \phi_l^1(x, y),
\end{aligned} \tag{8}$$

$$\{-\partial_x^2 - \partial_y^2 + v(x)\}\phi_l^2(x, y) + v(x)\phi_l^2(y, x) = \varepsilon_2^l \phi_l^2(x, y).$$

The set of functions $\{\psi_l^i\}$ biorthogonal to the set $\{\phi_l^i\}$ consists of the eigenfunctions of the equations adjoint to the Eq. (8)

$$\begin{aligned}
\{-\partial_x^2 - \frac{3}{4}\partial_y^2 + v(x)\}\psi_l^1(x, y) + \int_{-1}^1 dv \frac{xy}{x_1 y_1} v(x_1) \psi_l^1(x_1, y_1) = \\
= \varepsilon_1^l \psi_l^1(x, y),
\end{aligned} \tag{9}$$

$$\{-\partial_x^2 - \partial_y^2 + v(x)\}\psi_l^2(x, y) + v(y)\psi_l^2(y, x) = \varepsilon_2^l \psi_l^2(x, y).$$

A biorthogonal basis is required because the Faddeev operator is not self-adjoint¹⁶. Substituting (7) into the Eq. (6) and projecting onto conjugated basis $\{\psi_l^i\}$ we obtain the set of integro-differential equations for the functions $F_l^i(z)$, describing the relative motion of clusters

$$\begin{aligned}
& \{-\frac{2}{3}\partial_z^2 + \varepsilon_1^l - \varepsilon\}F_l^1(z) = \\
& = -\frac{1}{2} \sum_{k=0}^{\infty} \left\langle \psi_l^1(x, y) | v(x) \int_{-1}^1 du \int_{-1}^1 dv \left\{ \frac{xyz}{x_2 y_2 z_2} \phi_k^1(x_2, y_2) F_k^1(z_2) + \right. \right. \\
& \quad \left. \left. + \frac{xyz}{x_3 y_3 z_3} \phi_k^2(x_3, y_3) F_k^2(z_3) \right\} \right\rangle, \\
& \{-\frac{1}{2}\partial_z^2 + \varepsilon_2^l - \varepsilon\}F_l^2(z) = \\
& = -\sum_{k=0}^{\infty} \left\langle \psi_l^2(x, y) | v(x) \int_{-1}^1 dv \frac{xyz}{x_4 y_4 z_4} \phi_k^1(x_4, y_4) F_k^1(z_4) \right\rangle.
\end{aligned} \tag{10}$$

In these equations $\langle . | . \rangle$ means the integration over the variables x and y . The functions $F_l^i(z)$ must vanish when $z \rightarrow \infty$

$$F_l^i(z) \sim 0, \quad i = 1, 2, \quad l = 1, 2, \dots, \infty.$$

The number of equations in the set depends on the number of the terms retained in the expansion of the Yakubovsky components, Eq. (7). Due to completeness of the set of the basic functions only a finite number N of such terms needs to be taken into account to support a stable numerical solution.

IV. RESULTS

The solution of the Eq. (10) has been computed in the region Ω of the configuration space defined by the parameters R_x, R_y, R_z :

$$\Omega = \{x, y, z : x < R_x, y < R_y, z < R_z\}.$$

The values of these parameters were chosen to be $R_x=R_y=R_z=50$ Å. All the calculations were performed using model potentials HFDHE2⁷ and HFD-B⁸. From the one hand according to contemporary point of view these potentials give lower and upper limits for two-body binding energies correspondingly, and from another hand some four-body results for these potential models are known in literature²⁴.

The basic functions $\phi_l^i(x, y), \psi_l^i(x, y), i = 1, 2, l = 1, 2, \dots, N$ were calculated using the CRM¹⁸. To confirm the accuracy of the basic functions we were checking the basis for orthogonality using the condition

$$(\langle \phi_l^i | \psi_m^i \rangle - \delta_{lm}) < 10^{-3}, \quad i = 1, 2.$$

The function $\phi_1^1(x, y)$ for $l = 1$ and $k = 1$ in the Eq. (7) is the s -wave Faddeev component of the ground state wave function of the He₃ system (trimer). The binding energy of the He₃ ground state when computed for the HFDHE2 and the HFD-B potentials has the values -0.105 K and -0.118 K. Compared to the values reported by Carbonell et al.²¹ and Kolganova et al.²² our trimer is slightly overbound.

The He₄ (tetramer) binding energy, which has been computed using the potentials HFDHE2 and HFD-B, is given in the Tab. 1. In the same table we also quote the result reported by Nakaichi-Maeda and Lim²⁴. These authors used the formalism of integral AGS equations²⁵. In addition we include the results of the calculations of the mean square radius ($\langle r^2 \rangle^{1/2}$) of the system, the mean square distance between Helium atoms, and the probability of forming the subsystem with cluster structure He₃ + He. This last probability has been computed as

$$P_{3+1} = \langle \psi_1 F_1 | \Psi \rangle, \quad (11)$$

where Ψ is the total wave function of the system, ψ_1 is the ground state wave function of He_3 and F_1 is the function describing the motion of He_3 trimer relative to a single He atom. As can be seen from the table, the contribution of the $\text{He}_3 + \text{He}$ state to the total wave function is considerable.

The fast convergence of the cluster decomposition, Eq. (7) indicates the existence of clusters in subsystems. Particularly, in the 3+1 subsystem one needs to take into account two terms to get a stable binding energy. The binding energy computed by taking into account only the 3+1 component has the value -0.25 K, which is in good agreement with the value -0.24 K by Nakaichi-Maeda and Lim²⁴. To achieve a binding energy calculation that is stable at the scale 10^{-2} K one needs to take into account six terms in the Eq. (7) which use components of both types (3+1) and (2+2).

The analysis of the results of our computation of the characteristics of He_3 and He_4 systems enables us to draw an analogy with the nuclear cluster systems 3α and 4α . Here the symbol α denotes a ^4He nucleus. The bound states of these systems correspond to the ground states of nuclei ^{12}C and ^{16}O , respectively. It was known (for example^{17,26}) that in these cases the three-body systems have no well defined clusters in their subsystems. However, in the four-body systems the cluster of 3+1 type is dominant i.e. in this case it is possible to separate a closely bounded cluster of three particles and fourth particle. The mean square radius of the nuclear systems 3α ($\langle r^2 \rangle^{1/2} = 2.33$ fm) and 4α ($\langle r^2 \rangle^{1/2} = 2.54$ fm)¹⁷ increases with the number of particles. The situation is similar for the system under consideration. In particular for the potential HFDHE2 (HFDH-B) the mean square radius of trimer is 6.7 Å (6.5 Å) and that of the tetramer is 7.4 Å (6.9 Å) for the same potentials.

To characterize the spatial distribution of the particles constituting the tetramer we have computed its wave function (4) for the HFDHE2 potential. The density function $\rho(r)$ is depicted in Fig. 1. normalized with the usual condition $\int_0^\infty \rho(r) dr = 1$.

To study the spatial position of the Helium atoms in the tetramer we have used the total

wave function of the system. For comparison analogous calculations were performed for the trimer. The He_4 (He_3) wave function depends on six (three) variables. These are moduli of the Jacobi coordinates x, y, z (x, y) and cosines of the angles between vectors $\mathbf{x}, \mathbf{y}, \mathbf{z}$ (\mathbf{x} and \mathbf{y}) $u = \frac{(\mathbf{x}, \mathbf{y})}{xy}$, $v = \frac{(\mathbf{x}, \mathbf{z})}{xz}$, $w = \frac{(\mathbf{y}, \mathbf{z})}{yz}$. The most probable configurations of the relative position of the particles forming the He_4 (He_3) system was calculated as the coordinates of the maximum of the square of the total wave function. For He_3 system we found $x=3.6 \text{ \AA}$, $y=3.1 \text{ \AA}$, $u=0$, and for He_4 system $x=3.6 \text{ \AA}$, $y=3.1 \text{ \AA}$, $z=2.9 \text{ \AA}$, $u=0$, $v=0$, $w=0$. These configurations are shown in Fig. 2. For the ground state of the trimer the center of the He atoms masses arrange themselves at the vertices of the equilateral triangle with sides as large as 3.6 \AA (Fig. 2. a). For the ground state of the tetramer the three Helium atoms are located at the vertices of an equilateral triangle with sides as large as 3.6 \AA , while the most probable position of the fourth Helium atom is at a distance of 2.9 \AA in the direction perpendicular to the plane of the three particle system (Fig. 2. b) and through the center of the equilateral triangle formed by them. One should not be surprised by the predominance of the tetrahedron configuration if one takes into consideration the identity of particles and the s -wave approach that has been used for the description of the tetramer. One can compare the location of density function maximums with the positions of potential energy minimums. These positions differ noticeably that demonstrate the essentially quantum nature of the system. The minimums of potential forms a configuration of equilateral tetrahedron with the side of 3.0 \AA whereas the maximums of density function are located on the vertices of tetrahedron with the side of 3.6 \AA .

V. CONCLUSION

By applying the method of cluster reduction we have solved numerically the s -wave differential equations for the Yakubovsky components for a system with four ^4He atoms. Binding energy, mean-square radius and density function are calculated for the ground state. The results of the calculations are in good agreement with those of Nakaichi-Maeda

and Lim²⁴, which were performed using the integral equations. The configurations with He₃ cluster and separated helium atom dominates in the He₄ cluster. This behavior is analogous to that of the nuclear 4α particles system¹⁷. The most probable spatial configuration of the four Helium atom system is the tetrahedron with sides as large as 3.6 Å.

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FIGURES

FIG. 1. The comparison of the probability densities for three- and four He atom system: solid curve corresponds to the ground state of the He_4 system, dashed curve corresponds to the ground state of the He_3 system (HFDHE2 potential).

FIG. 2. The most probable configurations of Helium atoms: a) the ground state of the He_3 system, b) the ground state of the He_4 system. The figures show the numbers of atoms and distances between their centers of mass (HFDHE2 potential).

TABLES

TABLE I. $^4\text{He}_4$ tetramer binding energy (E_4), mean-square radius ($\langle r^2 \rangle^{1/2}$), mean square distance between Helium atoms ($\langle x^2 \rangle^{1/2}$) and the contribution of cluster subsystems of the $\text{He}_3 + \text{He}$ form (P_{3+1}).

Potential	HFDHE2		HFD-B
	present work	S. Nakaichi-Maeda and T.K. Lim ²⁴	present work
E_4 , K	-0.39	-0.394	-0.41
$\langle r^2 \rangle^{1/2}$, Å	7.4	—	6.9
$\langle x^2 \rangle^{1/2}$, Å	11.1	—	10.3
P_{3+1}	0.75	—	0.81